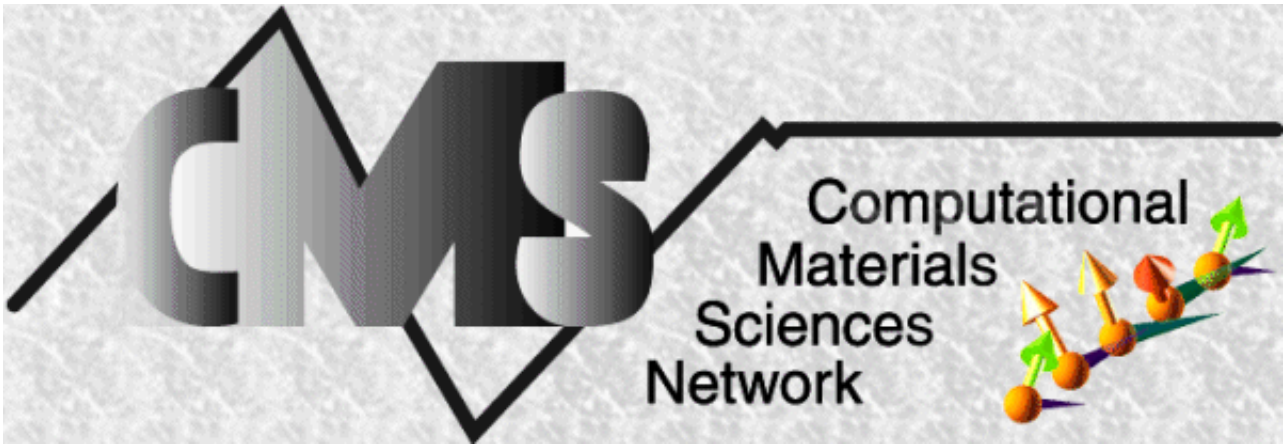

Volume 1, No. 1 **September 2000**

Welcome to the premiere issue of the Computational Materials Sciences Network (CMSN) newsletter!

The tremendous progress and promise of computation materials science is creating demands and opportunities for expanding research into new frontiers. Many of the most exciting new areas involve the study of highly complex materials or phenomena where rapid progress can be accelerated by teams of researchers. With these ideas in mind the DOE Division of Materials Sciences (Office of Basic Energy Sciences) this past year initiated the Computational Materials Sciences Network (CMSN) with the mission to advance the frontiers of computational materials science by assembling diverse sets of researchers committed to working together to solve outstanding materials problems that require cooperation across organizational and disciplinary boundaries. The intent of the modest "glue money" for CMSN is to foster partnering and collective activities among members of collaborative research teams (CRTs). There are currently five CRTs within CMSN. A brief overview of each of their projects is presented in the next section. This newsletter is one mechanism to share the collective research efforts of the CMSN projects with all the CRT participants and with the larger CMS community. As the research of the CRTs advances, progress reports and highlights of the scientific results will be featured in future issues of the newsletter. Other items pertaining to the development of the CMS community will also be included. Ideas for such items are welcomed.

The CMSN web pages contain a database of network associates (from which the mailing list of this newsletter is obtained) and also information about the CRT projects, workshops, and job opportunities. To add your name to the associates database, please fill out the form available at http://cmpweb.ameslab.gov/ccms/associate.html. The current coordinators of CMSN are listed below, and they may be contacted with questions, comments or suggestions regarding CMSN.

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Project Overviews

Microstructural Evolution Based on Fundamental Interfacial Properties

Principal Investigators: Tony Rollett,Carnegie Mellon Univesity, David Srolovitz, Princeton University

Overview: There are two main streams of activity in materials science. The first, materials discovery, is based either on serendipity and/or Edisonian research. The second, material optimization, is ideally based upon our understanding of the relationship between composition, structure and properties and our ability to process materials to achieve target compositions and structure. While materials discovery is inherently fascinating and important, it is the area of materials optimization that presents the greatest opportunities. Arguably, the most important applications of advances in computational power and algorithms to materials science has been in the area of materials optimization, in general, and materials processing, in particular. These advances have primarily been in the area of application of continuum methods for matter and heat transport. These models typically invoke empirical constitutive relations to describe how a material will behave. As a result, these methods can be routinely used to predict the final shape of a specimen following deformation processing and its temperature history, but is of little use in determining, predicting, or manipulating the internal structure or microstructure of the material. It is the microstructure that controls the properties of a material and it is the primary knob that we materials scientists and engineers have at our disposal to optimize material properties. For more details about this project, visit the Web site **http://cyclops.ameslab.gov/cmsn/**

Microstructural Effects on the Mechanics of Materials

Principal Investigators: Richard LeSar, Los Alamos National Laboratory Dieter Wolf, Argonne National Laboratory

Overview This team brings together a diverse set of researchers, each with their own approaches and skills, to develop a hierarchically structured, integrated approach towards materials modeling across all the inherent physical length and time scales relevant to microstructural effects in materials mechanics. To focus the efforts of the team, we investigate the interplay between dislocation and grain microstructures in polycrystal plasticity. Our specific goal is to elucidate the fundamental dislocation and grain-boundary processes thought to be responsible for the crossover in the well-known Hall-Petch effect, from “normal” behavior at larger grain sizes to the “inverse” behavior for grain sizes less than typically 20 nm in grain size. Insights gained from this study will naturally lead to a better understanding and predictive capability for related, but more complex deformation processes in polycrystalline materials, such as superplastic forming of metals and ceramics. By focusing the efforts of a variety of researchers with broad scientific and computational expertise on the same problem, perhaps the most important outcome of this team effort will not only be the development of a conceptual framework enabling the bridging of lengthand time scales in materials modeling but also the emergence of new scientific ideas and more predictive models in this important area of materials science. The Web page is **http://www.msd.anl.gov/im/cmsn/cmsn.html**

Polymers at Interfaces

Principal Investigator: Gary S. Grest, Sandia National Laboratory

Overview: Interfaces between polymers and hard surfaces, such as ceramics and metal oxides, dominate many properties of composite materials and coatings. The proposed research would build a fundamental understanding of how chemical bonding between these dissimilar materials at the atomic level determines macroscopic properties such as structure, adhesion, friction, stiffness, fracture toughness, and chemical stability. This will require linking a variety of calculational techniques designed for different materials and different length scales.

Magnetic Materials Bridging Basic and Applied Science

Principal Investigators: Malcolm Stocks, Oak Ridge National Laboratory
Bruce Harmon, Ames Laboratory

Overview: While the underlying mechanisms responsible for the magnetism of materials involve electronic interactions at the atomic level, the bulk properties of permanent magnets are governed at a larger length scale and are greatly influenced by microstructure. The magnetics literature (probably from the time of the ancient Greeks) is rich in recipes for enhancing magnet performance by modifying the microstructure during processing (sometimes by rather crude heat and beat techniques). The magnetics communities are now in position to better understand and control the relevant microstructure for optimizing magnet performance. High performance computing is enabling researchers to model magnetic devices at smaller and smaller length scales, while at the same time accurate first principles calculations of magnetic properties now extend to systems involving thousands of atoms. The two different approaches: continuum versus discrete, and physics versus engineering, are approaching each other at mesoscopic length scales. There is a great opportunity to bring both communities together, and that is the goal of this project. The five subtasks of this project are: 1) Fundamental Physics, 2) First Principles derived parameters, 3) Domain Walls, 4) Coarse Graining, and 5) Micro-magnetics Code Development. Approximately 25 scientists from DOE labs, universities, other government laboratories, and industry are involved in one or more of the subtasks.

Excited-State Electronic Structure and Response Functions

Principal Investigators: Steven Louie (Univ. of California, Berkeley)
John Rehr (Univ. of Washington)

Overview: Many important materials science applications (e.g. microelectronic devices, optics, solar cells, and semiconductor lasers) depend, for their functionality, on electronic excited-state properties of materials. Likewise, most experimental probes create excitations and consequent materials' response. Modern photon sources (synchrotrons, ultra-fast lasers, etc.) now probe materials with unprecedented resolution and offer the potential for novel materials stud-

ies. In recent decades, computational physics has achieved enormous successes in describing ground-state properties; however, quantitative and reliable descriptions of excitations and response functions are just emerging. The objective of the proposed cooperative research team (CRT) is to attack these challenging, but timely, scientific and computational issues. The proposal has specific short- and long-term objectives, aimed at creating a deeper theoretical understanding through predictive calculations of materials' properties involving excited states. Our effort naturally breaks into three interconnected parts, a) experimental processes and applications; b) fundamental electronic excitations and correlations; and c) time-dependent phenomena and non-linear effects. We plan to develop compatible computational tools that can be shared between groups in a way that fosters parallel, interrelated, and compatible efforts. The project Web page found at **http://www.phys.washington.edu/%7Ejjr/Cmsn/cmsn.html**

Extended Abstract

Polymers at Interfaces

Gary S. Grest, Sandia National Laboratory

The role of polymer composites and coatings in industrial applications is rapidly growing due to their strength, light weight, chemical stability and tailorability. In these systems, the main area of concern is often the interface between the polymer and a hard surface. This is because the interface is the major locus for initiation of mechanical and chemical failure - the weak link in the chain. Examples where the interface plays an important role include the structural adhesives used in aerospace and automotive applications, paints and coatings, the photo-resist and other polymers used in microelectronics, barrier coatings used in food packaging, and the photo-receptor layers coated on a metallic drum in small photocopiers and laser printers. A poorly designed interface has negative consequences in all of these cases: an adhered joint could fall apart, a food product could become contaminated, the computer chip or photocopier could cease functioning correctly.

Understanding the nature of the interface between dissimilar materials poses a number of scientific challenges. One first must understand the chemical bonding between sites on oxide surfaces and the many different chemical components of typical polymers. These must then be used to develop atomistic interaction potentials that simultaneously describe interfacial interactions, the strong covalent bonds within oxides and individual polymers, and the weaker bonds that allow polymers to express conformational degrees of freedom. These degrees of freedom allow a rich variety of chemical and morphological changes in the polymer as a function of the distance from the interface. These have been explored for simple non-specific interfacial interactions, but the more complicated interactions with oxides may lead to a wealth of more intricate interfacial structures. Processes which may be important include, but are not limited to, selective absorption of polymer matrix components or additives, penetration of the polymer components into the second phase, such as would occur in polymer/fiber composites, diffusion of low molecular weight components from the interface into the polymer matrix, surface induced or surface modified crystallization of the polymer, and catalytic effects of the surface on the polymer matrix. Understanding the atomic origins of these effects, and developing predictive tools is a major scientific challenge.

One reason that adhesion and failure are difficult to predict is that the failure process is highly non-linear and does not depend simply on

the number and strength of local bonds. Redistribution of stress as bonds fail can change the location of failure or produce complex structures such as branching cracks or polymer crazes. Stress and chemical attack can also act synergistically to produce failure. Under shear failure produces sliding within the polymer or at the interface and thus involves friction. Polymers are frequently used to lower or raise friction to create improved energy efficiency or traction, but there is little molecular-level understanding of the factors that control friction. An important goal of our project is to understand the complex connections between atomic properties and the mechanisms of failure. That is, what is the connection between atomic bonding, geometry, and macroscopic friction?

Many systems have large numbers of interfaces between different components. This may occur through mixing of particles in a polymer to make a composite, or through segregation of different components due to equilibrium phase separation or non-equilibrium driving forces. For polymer/polymer and polymer/fiber composites, the interface is strongly affected by miscibility on the microscopic scale. At the simplest level one may consider copolymers or surfactants that concentrate at interfaces to improve adhesion or friction. These and other additives may also produce intricate domain structures in polymer blends that affect macroscopic properties. Some of the most dramatic effects are observed in polymer/clay composites where the mechanical, thermal, and interfacial properties of a polymer matrix can be dramatically improved by adding fillers. For example, the addition of just a few weight percent of an inorganic filler can often double the tensile strength and modulus and triple the heat distortion temperature of polymer/clay composites.

Progress on the issues described above will impact nearly every facet of American industry. The results could lead to improved products, such as paints, adhesives, lubricants, tires and composites. Understanding the relation between molecular structure and macroscopic properties could also speed the selection of chemicals for new applications.

To address the complex scientific problems described above we have assembled a team that brings together expertise in the disparate materials and length scales that must be addressed. Recently, there has been substantial advances in materials modeling for both soft materials, such as polymers and foams, and hard materials, such as ceramics and metal oxides. The present research team is the first to bridge the gap between the communities working on these two classes of materials, and create new models for interfacial potentials. The ultimate scientific goal of our project is an understanding of how the atomic-scale chemical bonding at polymer interfaces controls macroscopic properties. This will require coherent scientific advances on a number of fronts, ranging from the chemistry of polymer/oxide bonds to the failure mechanisms at interfaces and in bulk to diffusion at interfaces to microstructure evolution during processing.

Highlight of this Issue

Anisotropic Interfacial Properties and their Effect on Microstructural Evolution

A. D. Rollett, A. Karma and D. J. Srolovitz
Carnegie Mellon University
Northeastern University
Princeton University

Motivation - The processing of materials to obtain specific microstructures and thus the desired material properties is a very general aspect of the materials industry. It is a predominantly empirical activity although there are many examples of the application of scientific understanding to the development of processing. One classic example is the development of technology for casting single crystal blades in superalloys for gas turbine engines, based on either the control of dendritic growth available through directional solidification, or the directional solid-state coarsening of the grain structure. This application is just one of many examples in which the migration of interfaces controls the microstructural evolution *and in which the anisotropy of the interfaces is critical to the process*. As the example illustrates, both solid-liquid and solid-solid interfaces are important: both have significant anisotropies in their energy and mobility. In fact, there is a sizeable and growing activity called Grain Boundary Engineering (GBE) that seeks to exploit the anisotropy of homophase boundaries in order to optimize properties such as stress-corrosion resistance and creep resistance.

The first year has seen exciting developments in our understanding of the solid-liquid interface. A proposed method to extract the interfacial energy and its anisotropy from the equilibrium fluctuation spectrum of the solid-liquid interface has been successfully implemented in MD simulations. One key element of this implementation is an improved definition of the order parameter that distinguishes between the solid and liquid phases. The interface structure factor (mean-square amplitude of fixed wavenumber fluctuations) has been shown to be inversely proportional to the square of the wavenumber for different orientations of the solid-liquid interface, in agreement with theoretical expectation. For different orientations, the interfacial stiffness has been obtained by measuring the slope of the plot of the inverse of the structure factor versus wavenumber squared. The stiffnesses for the 100 and 110 orientations yielded a value of the solid-liquid interfacial energy for pure Ni that is consistent with existing theoretical estimates, and the first prediction of anisotropy (slightly below 2 percent). These results have been incorporated into studies of microstructural evolution using a 2D phase-field model that incorporates stochastic forces. Simulations show that both the microstructure and the envelope of the solidification front depend sensitively on the strength of thermal fluctuations in a way that remains poorly understood. More information and results can be found at **http://cmpweb.ameslab.gov/ccms/otherlinks/ssi/simulations.html**

The range of grain boundary types is rather large because even in a single phase material, a boundary has five degrees of (macroscopic) freedom. The energy of grain boundaries has been extensively investigated over the years although most of the information is confined to the energy and mobility of a few, highly symmetric boundary types. The motivation for performing extensive simulations of grain boundary properties, including energy, mobility and chemical segregation, is

to understand the formation of both special textures (e.g. the {001}<100> texture that is critical to formability in aluminum sheet) and special boundary character (as in GBE). We currently know that there are a few pronounced minima in g.b. energy and a few pronounced maxima in mobility. These features are related to, but not predicted by geometrical models of boundary structure (e.g the coincidence site lattice model). Very little is known about the interplay between g.b. type and chemical segregation: real materials, however, always have significant levels of solute present that strongly affect mobility.

Accomplishment - Molecular dynamics simulations of grain boundary migration in 3D have progressed to the point where a wide range of boundary types have been examined for tilt and twist boundaries in aluminum. Energies are extracted by evaluating the change in system energy with time. Reduced and intrinsic mobilities are extracted by measuring migration rates, just as in experiments. Significant anisotropies in energy and mobility have been quantified and found to have strong effects on grain growth in simulations of 2D polycrystals. The results are in good agreement with experimental date for mobility in aluminum. Special properties such as high mobility and low energy are found for boundaries near the $\Sigma 7$ and $\Sigma 13$ positions, as well as a 30° <111> boundary type. Enhanced computing power means that it is now feasible to calculate migration rates of realistic boundary configurations in atomistic simulations and extract boundary properties. Future work will examine the properties of less symmetric boundaries. Current results on grain boundary migration can be found at **http://safed.princeton.edu/Research/ThreeDimGB/CurResults.html**

Significance - The mapping of anisotropic interfacial properties over the very large space of boundary types (even for cubic materials) is vitally necessary information for accurate simulation of microstructural evolution. The set of boundaries being investigated has been determined by consideration of common boundary types that occur in the process of recrystallization in fcc metals such as aluminum. The ability to predict and control the recrystallization (and grain growth) process in metals such as aluminum will be of great technological value. The same methods will be extended to more complex materials such as the ferroelectric and piezoelectric oxides. There is a major effort underway in these materials, for example, to grow single crystals through sintering and grain growth using seed crystals. Although the method works, very little is known about the fundamental properties of the boundaries that permit it to occur and the simulation will be an essential tool for advancing our understanding of such processes.

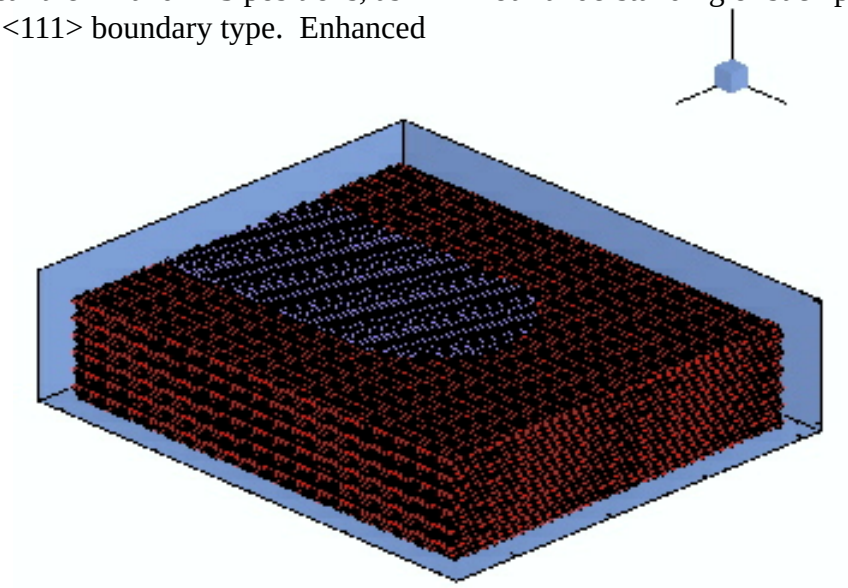

Fig. 1. Molecular dynamics simulation of bi-crystal with U-loop boundary to provide constant driving force; the boundary migrates so as to shrink the loop.

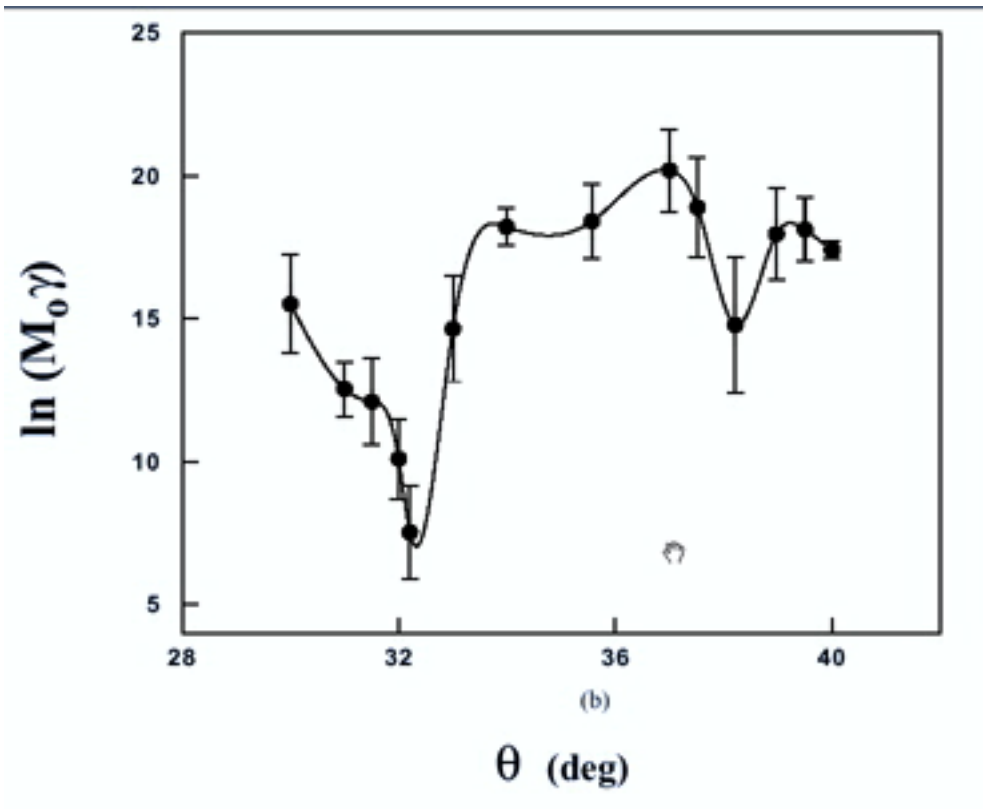

Fig. 2. Variation of (reduced) mobility versus angle for grain boundaries based on the <111> misorientation axis, showing significant cusps at two special orientations.

Workshop Report

by Dieter Wolf and Richard LeSar

FY 2000 Report on the CMSN Thrust on
"Microstructural Effects on the Mechanics of Materials" and on the *CMSN Workshop*
held at *ANL, June 5-7, 2000*

The main thrust of this team effort is the elucidation of the deformation behavior of polycrystalline materials by means of computer simulations, with particular emphasis on the elucidation of the interplay between dislocation and grain-boundary processes in polycrystal plasticity. For that purpose, a multiscale simulation approach incorporating all the relevant length and time scales involved in the deformation is being developed; this approach provides not only fundamental insight into the underlying atomic-level deformation mechanisms but also offers a quantitative description of how these mechanisms ultimately control the macroscopic deformation behavior as captured, for example, in constitutive relations. In this multiscale approach, the mesoscale, i.e., the length and time scales associated with the grain-boundary and dislocation microstructures and their dynamical interactions, provides the critical link between the atomic and continuum levels.

The ANL workshop served several purposes, each of which is critical to the success of this team effort. First, the workshop was necessary to further coordinate the four initially funded subtasks within our cooperative research team (CRT) and to update the team as a whole on any relevant developments and recent progress made within each subtask area since the formulation of the original team proposal. Second, it is essential that our multiscale simulation approach is well connected to similar multiscale simulation projects, such as DOD's ASCI program and the CMSN thrust on "Microstructural Evolution Based on Fundamental Interfacial Properties." Third, the workshop provided a forum for a concerted effort to better connect our computer modeling work with experiments; this connection is critical for the overall success of our simulation work. This report documents the present status of our CMSN team effort discussed extensively at the workshop. It concludes with a list of action items identified in the plenary discussion at the end of the workshop, and with our budget plan for FY 2001. The workshop program and a complete list of participants are attached to the end of this report. A limited number of copies of a compendium containing the viewgraphs presented at the workshop is available from the organizers upon request. Up-to-date information related to this team effort can be found at **http://www.msd.anl.gov/groups/im/cmsn/cmsn.html**. The full text of this report is available at **http://www.msd.anl.gov/IM/cmsn/FY2000report.html**.

Upcoming Conferences

October 2-6, 2000: 47th International AVS Symposium — Magnetic Interfaces and Nanostructures Division Hynes Convention Center, Boston, Mass.

Program Chair: C.R. Abernathy (University of Florida), caber@mse.ufl.edu

The Magnetic Interfaces and Nanostructures Division highlights recent scientific results and technological challenges in the areas of magnetic materials and devices. The continually growing interest in these fields derives from the development or discovery of new materials, new phenomena, novel magnetic or spin-sensitive devices, nanostructured media, and new techniques for the fabrication and study of magnetic thin films and heterostructures. A primary goal of the MI program is to elucidate the effects of surfaces and interfaces on the properties of media and devices that rely on magnetic materials for their functionality. The program integrates spectroscopic and imaging studies of growth, structure, and magnetization with a traditional emphasis on surface and interface magnetism as addressed by spin-resolved and magneto-optic techniques. Nascent device technologies, materials, and measurement techniques also will be addressed by invited speakers and contributed presentations in the MI sessions, some of which will be joint with NSTD, Nano-6 and EMPD.
Web site: http://divisions.vacuum.org/min/MINpage.html

November 13-14, 2000: Workshop on the Excited State Electronic Structure and Response Functions, Supercomputer Center, University of Minnesota, Minneapolis, Minn.

Local Organizer: Prof. James R. Chelikowsky

Many experimental probes of materials properties involve electronic excitations. Modern high intensity photon sources (synchrotrons, ultrafast lasers, etc.) can now probe materials with unprecedented resolution and open the potential for novel materials processing and materials science studies. In the last few decades, computational physics has achieved enormous successes in describing ground-state properties. In contrast, quantitative descriptions of excitations and response functions are just emerging. The objective of this workshop is to assess the technical and computational issues that will enable calculations of linear and nonlinear response functions at the same level of sophistication and accuracy that is now possible for the ground-state. Specific short- and long-term objectives that will impact theoretical understanding and applications to materials studies, including characterization and processing will be discussed and presented at this meeting.
Web site: http://www.msi.umn.edu/general/Symposia/Excited/

January 8-19, 2001: Pan-American Advanced Studies Institute on Computational Materials Science, Pontificia Universidad Católica de Chile, Santiago, Chile.

Computational Materials Science (CMS) is one of the broadest, most rapidly evolving and technologically significant areas of science today. From its foundations in basic science CMS branches to new materials, to processing, and to the life sciences. Due to rapid advances in computational capacity, including new algorithms, software macro-packages and low-

cost PC's, CMS problems previously thought intractable are actively being pursued. The enhanced capabilities of CMS are increasingly impacting the search for new materials, the improvement and design of processing techniques, and the research in bio-areas such as protein folding.

The rapid advances and interdisciplinary research taking place in CMS makes it an ideal subject for the Pan-American Advanced Studies Institute (PASI) which will feature a spectrum of forefront topics in this field. Progress in this field will be most rapid when scientists from a range of disciplines and subdisciplines are brought together on projects that require broad expertise not usually found in one group or organization. Students and postdocs in particular would benefit by extending their experience beyond their specialization and becoming familiar with the exciting progress being made in overlapping disciplines. The PASI conference will help establish networking contacts in related but crucial fields (including computer science and applied mathematics).
Web site: http://www.iitap.iastate.edu/iitap/pasi.html.

Job Openings

Postdoctoral Position at Argonne National Lab

The Interfacial Materials Group in the Materials Science Division at Argonne National Laboratory has a postdoctoral opening in the area of "Simulation of Plastic Deformation of Polycrystalline Materials," with emphasis on the interaction between dislocations and grain boundaries. The simulations will involve large-scale molecular-dynamics, Monte-Carlo and/or finite-element simulations. As part of an eight-member simulation team, the successful candidate will develop and use parallel computer codes (on Argonne's IBM-SP, the Cray T3E at NERSC and our new Beowulf cluster and extensively use graphics visualization and virtual reality tools (for example, in the Argonne CAVE). A Ph.D. in a theoretical discipline related to mechanical properties and experience with some aspect of atomistic, mesoscopic, or finite-element modeling is required. US citizenship is not required. Please send resume and names of three references to Dr. Dieter Wolf or Dr. Simon Phillpot, Materials Science Division, Bldg. 212, Argonne National Laboratory, Argonne, IL 60439.

Postdoctoral Opening at the Center for Computational Materials Science - Naval Research Laboratory

JOB DESCRIPTION: Further develop and apply density-functional-based methodologies to isolated and assembled molecular and cluster-based systems. Experience with one ore more electronic structure methods is required. Significant experience with UNIX, LINUX, FORTRAN, MPI is highly desireable.

A sample of current research interests:

MOLECULAR MAGNETISM: Calculations deal with determining equilibrium geometries, electronic structures, spin-ordering and anisotropy energies in clusters. High level density-functional

based calculations are also used to determine exchange parameters for Heisenberg Hamiltonians. Interests are in predicting spin-tunneling fields and on the computational enhancement of magnetic anisotropies. Recent calculations have been on the Mn12 and Fe8 spin-tunneling magnets, the V15 half integer spin system and on the Fe13O8 uniaxial magnetic clusters.
ENERGETIC MOLECULES: Calculations deal with electronic and vibrational spectra of energetic molecules. Examples of recent applications in this area include enclathrated gas molecules, octanitrocubane, azidopentazole and other nitrogen containing compounds.

METHODOLOGIES: Present interest is in incorporating spin-orbit interactions and other relativistic interactions into standard electronic structure programs and in including many-body corrections to the density-functional theory.

Interested candidates please contact Mark R. Pederson, Code 6392, Naval Research Laboratory, Washington DC 20375-5345. NRL is an EEO/AA Employer.

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Editor and Webmaster: Sreeparna Mitra
Web Page:http://cmpweb.ameslab.gov/ccms/